

11/602,551

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:asptal20ltxs

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOKCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and IMEDLINE reloaded with enhancements
NEWS	9	FEB 08	STN Express, Version 3.3, now available
NEWS	10	FEB 20	PCI now available as a replacement to DPCI
NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDS, IFLEAT, and IFIUDS enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/CAPLUS and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LOPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMEASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	21	APR 28	EMEASE Controlled Term thesaurus enhanced
NEWS	22	APR 28	IMSRESEARCH reloaded with enhancements

NEWS EXPRESS FEBRUARY 08 CURRENT WINDOWS VERSION IS V8.3,
AND CURRENT DISCOVER FILE IS DATED 20 FEBRUARY 2008

NEWS HOURS STN Operating Hours Plus Help Desk Availability
NEWS LOGIN Welcome Banner and News Items

11/602,551

NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN Customer agreement. Please note that this agreement limits use to scientific research. Use for software development or design or implementation of commercial gateways or other similar uses is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 14:24:27 ON 10 MAY 2008

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 14:24:50 ON 10 MAY 2008

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 9 MAY 2008 HIGHEST RN 1020227-00-2

DICTIONARY FILE UPDATES: 9 MAY 2008 HIGHEST RN 1020227-00-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\Stnexp\Queries\116025511.str



```

chain nodes :
6 7 8 9 11 13 15 16
ring nodes :
1 2 3 4 5
chain bonds :
2-6 3-13 4-9 5-15 5-16 6-7 6-8 8-11
ring bonds :
1-2 1-5 2-3 3-4 4-5
exact/norm bonds :
3-13 4-9 5-15 5-16 6-7 6-8 8-11
exact bonds :
1-2 1-5 2-3 2-6 3-4 4-5
isolated ring systems :
containing 1 :

```

11/602,551

G1:H,Ak

G2:H,X,Ak

G3:Cb,Ak,H

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS
11:CLASS 13:CLASS 15:CLASS 16:Atom

L1 STRUCTURE UPLOADED

=> s 11

SAMPLE SEARCH INITIATED 14:25:08 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 161 TO ITERATE

100.04 PROCESSED 161 ITERATIONS 7 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
MATCH **COMPLETE**
PROJECTED ITERATIONS: 2459 TO 3981
PROJECTED ANSWERS: 7 TO 298

L2 7 SEA SSS SAM L1

=> s 11 ful

FULL SEARCH INITIATED 14:25:14 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 2853 TO ITERATE

100.04 PROCESSED 2853 ITERATIONS 106 ANSWERS
SEARCH TIME: 00.00.01

L3 106 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	178.36	178.57

FILE 'CAPLUS' ENTERED AT 14:25:24 ON 10 MAY 2008
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available

11/602,551

for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1967 - 10 May 2008 VOL 148 ISS 20
FILE LAST UPDATED: 9 May 2008 (20080509/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

<http://www.cas.org/infopolicy.html>

=> s 13

L4 42 L3

=> d 14 ibib hitstr abs 1-42

L4 ANSWER 16 OF 42 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2003:926825 CAPLUS
DOCUMENT NUMBER: 140:228444
TITLE: Quantitative relationship between rat intestinal
absorption and Abraham descriptors
AUTHOR(S): Zhao, Yuan H.; Abraham, Michael H.; Hersey, Anne;
Luscombe, Chris N.
CORPORATE SOURCE: Department of Chemistry, University College London,
London, WC1E 6AJ, UK
SOURCE: European Journal of Medicinal Chemistry (2003),
38(11-12), 939-947
CODEN: EJMCA5; ISSN: 0223-5234
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
IT 72420-38-3, Acifran
EL: PKT (Pharmacokinetics); PRP (Properties); THU (Therapeutic use);
BIOL
(Biological study); USES (Uses)
(quant. structure-activity relationship (QSAR) between rat
intestinal
drug absorption and Abraham descriptors)
RN 72420-38-3 CAPLUS
CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl- (CA INDEX
NAME)



AB Literature data on the intestinal absorption of 158 drug and drug-like compds. in rats have been collected, and Abraham descriptors for the set

of drugs have been calculated using the method of Platts and Abraham et al.

Results show that there is a significant relationship between rat intestinal absorption and the Abraham descriptors. In agreement with the

human intestinal absorption model, the dominant descriptors in the rat model are the drug hydrogen bond acidity and basicity. In order to compare the absorption models in humans and rats, the absorption model developed from rats was used to predict the absorption in humans. The rat

intestinal absorption model is similar to the human absorption model, and

data on rats can effectively be used to predict human intestinal absorption.

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE
FORMAT

14 ANSWER 29 OF 42 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:587086 CAPLUS

DOCUMENT NUMBER: 121:187086

ORIGINAL REFERENCE NO.: 121:33849a, 33852a

TITLE: NMR studies of drugs. Applications of achiral and chiral lanthanide shift reagents to acifran methyl ester. LSR binding to a multifunctional substrate

AUTHOR(S): Gray, Lovett; Rothchild, Robert

CORPORATE SOURCE: John Jay Coll. Criminal Justice, City Univ. New York,

New York, 10019-1199, USA

SOURCE: Spectroscopy Letters (1994), 27(7), 935-54

CODEN: SPLEBK; ISSN: 0038-7010

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 72429-82-4P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(achiral and chiral NMR lanthanide shift reagents binding to
acifran Me
ester)

11/602,551

RN 72429-82-4 CAPLUS

CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl-, methyl ester
(CA INDEX NAME)



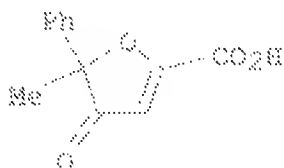
IT 72420-38-3, (±)-Acifran

RE: RCT (Reactant); RACT (Reactant or reagent)

(esterification; achiral and chiral NMR lanthanide shift reagents binding to acifran Me ester)

RN 72420-38-3 CAPLUS

CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl- (CA INDEX NAME)



AB The NMR spectra of (±)-acifran Me ester was studied by using achiral and chiral Europium shift reagents [e.g., Slever's reagent, Eu(HFC)3] for potential determination of enantiomeric excess. The shift magnitudes were interpreted as consistent with major lanthanide binding at the 4-oxo carbonyl of the mol.

L4 ANSWER 38 OF 42 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1982:527417 CAPLUS

DOCUMENT NUMBER: 97:127417

ORIGINAL REFERENCE NO.: 97:21145a,21148a

TITLE: Hypolipidemic

4,5-dihydro-4-oxo-5,5-disubstituted-2-furancarboxylic acids

AUTHOR(S): Jirkovsky, Ivo; Cayen, Mitchell W.

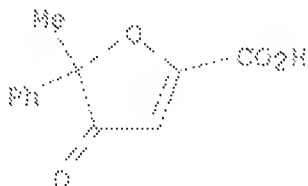
CORPORATE SOURCE: Biochem. Dep., Ayerst Lab., Montreal, QC, H3C 3J1, Can.

SOURCE: Journal of Medicinal Chemistry (1982), 25(10), 1154-6

11/602,551

CODEN: JMCMA8; ISSN: 0022-2623
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 97:127417
IT 77103-94-7P
RL: SPN (Synthetic preparation); PPEP (Preparation)
(preparation and conversion to free base)
RN 77103-94-7 CAPLOS
CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl-, (+)-,
compd.
with (R)- α -methylbenzenemethanamine (1:1) (9CI) (CA INDEX NAME)
CM 1
CBN 77103-91-4
CMF C12 E10 O4

Rotation (+).



CM 2
CBN 3886-69-9
CMF C8 E11 N

Absolute stereochemistry. Rotation (+).



IT 77154-54-2P
RL: SPN (Synthetic preparation); PPEP (Preparation)
(preparation and free base from)
RN 77154-54-2 CAPLOS
CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl-, (-)-,
compd.
with (S)- α -methylbenzenemethanamine (1:1) (9CI) (CA INDEX NAME)
CM 1
CBN 77103-92-5

II/50C, 551

CMF C12 H10 O4

Rotation (-).



CM 2

CPN 2627-86-3

CMF C8 H11 N

Absolute stereochemistry. Rotation (-).



IT 72420-38-3P 72420-40-7P 72429-82-4P
77103-87-8P 77103-91-4P 77103-92-5P

RL: BAC (Biological activity or effector, except adverse); BSU

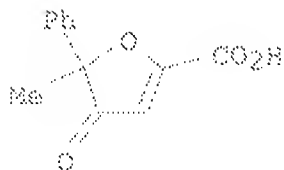
(Biological

study, unclassified); SPN (Synthetic preparation); BIOL (Biological
study); PREP (Preparation)

(preparation and hypolipidemic activity of;

RN 72420-38-3 CAPLUS

CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl- (CA INDEX
NAME)



RN 72420-40-7 CAPLUS

CN 2-Furancarboxylic acid, 4,5-dihydro-5-(1-methylethyl)-4-oxo-5-phenyl-
(CA INDEX NAME)

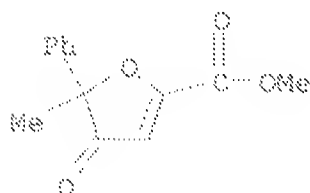
11/602,551



PN 72429-82-4 CAPLUS

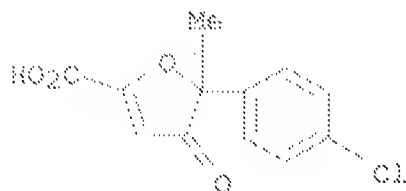
CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl-, methyl ester

(CA INDEX NAME)



PN 77103-87-8 CAPLUS

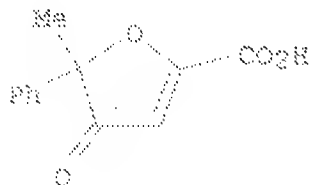
CN 2-Furancarboxylic acid, 5-(4-chlorophenyl)-4,5-dihydro-5-methyl-4-oxo-
(CA INDEX NAME)



PN 77103-91-4 CAPLUS

CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl-, (+)- (CA INDEX NAME)

Notation (+).

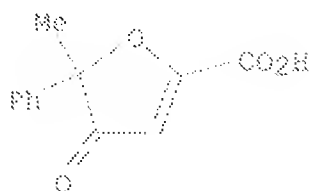


PN 77103-92-5 CAPLUS

CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl-, (-)- (CA INDEX NAME)

11/602,551

Rotation (-).



GI



AE Cyclocondensation of $RR_1C(OH)COMe$ (P, $R_1 = Me, Me; Me, Ph; Me, Me_2CH, Ph$; $RR_1 = 3,4$ -dihydro-1(2H)-naphthalenyldiene) with EtO_2CCO_2Et gave furancarboxylic acids I. I ($R, R_1 = Me, Ph$) showed hypolipidemic activity superior to that of nicotinic acid and clofibrate.

L4 ANSWER 40 OF 42 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 1980:41746 CAPLUS
DOCUMENT NUMBER: 92:41746
ORIGINAL REFERENCE NO.: 92:6961a,6964a
TITLE: 4,5-Dihydro-4-oxofuran-2-carboxylic acid
derivatives
INVENTOR(S): Jirkovsky, Ivo L.; Dvornik, Dusan; Cayen,
Mitchell N.
PATENT ASSIGNEE(S): American Home Products Corp., USA
SOURCE: U.S., 10 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4169202	A	19790925	US 1978-312798	19780605
AU 7946892	A	19791213	AU 1979-46892	19790509

11/602,551

AD 537177	B2	19840614		
US 4244958	A	19810113	US 1979-38028	19790510
EP 6305	A1	19800109	EP 1979-300926	19790524
EP 6305	B1	19820811		
R; AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AT 1449	T	19820815	AT 1979-300928	19790524
WO 8000025	A1	19800110	WO 1979-US376	19790529
W; DK, JP, SU				
JP 55500473	T	19800731	JP 1979-500920	19790529
JP 01008629	B	19890214		
CA 1118777	A1	19820223	CA 1979-328790	19790531
ZA 7902773	A	19810128	ZA 1979-2773	19790603
HU 22733	A2	19820628	HU 1979-AE575	19790605
HU 180199	B	19830228		
DK 8000375	A	19800129	DK 1980-375	19800129
DK 165005	B	19920928		
DK 165005	C	19930208		
PRIORITY APPLN. INFO.:			US 1978-912798	A 19780605
			EP 1979-300928	A 19790524
			WO 1979-US376	W 19790529

OTHER SOURCE(S): MARPAT 92:41746

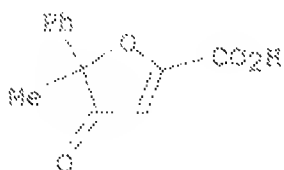
IT 72420-38-3P

PL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation);
 RACT (Reactant or reagent)

(preparation and esterification of)

RN 72420-38-3 CAPLOS

CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl- (CA INDEX NAME)



IT 72420-39-4P 72420-40-7P 72420-44-1P

72420-45-2P 72420-46-3P 72420-49-6P

72429-62-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 72420-39-4 CAPLOS

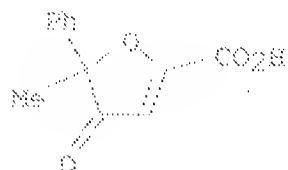
CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl-, compd.
 with benzenemethanamine (1:1) (SCI) (CA INDEX NAME)

11/602,551

CM 1

CRN 72420-38-3

CMF C12 H10 O4



CM 2

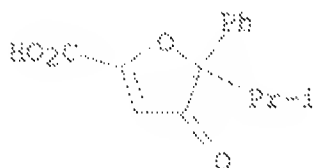
CRN 100-46-9

CMF C7 H9 N

B2N-CH2-Ph

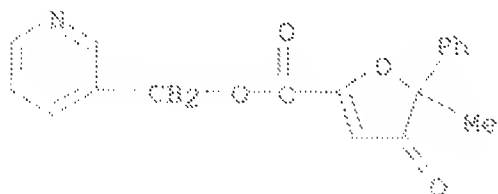
RN 72420-40-7 CAPLUS

CN 2-Furancarboxylic acid, 4,5-dihydro-5-(1-methylethyl)-4-oxo-5-phenyl-
(CA INDEX NAME)



RN 72420-44-1 CAPLUS

CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl-,
3-pyridinylethyl ester (CA INDEX NAME)



RN 72420-45-2 CAPLUS

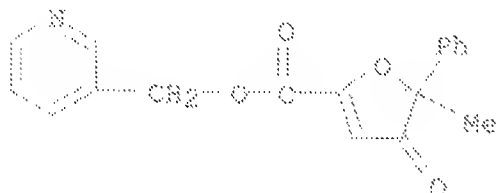
11/602,551

CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl-,
3-pyridinylmethyl ester, (2E)-2-butenedioate (2:1) (9CI) (CA INDEX
NAME)

CM 1

CEN 72420-44-1

CMF C18 H15 N O4

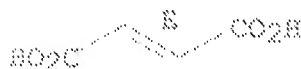


CM 2

CEN 110-17-8

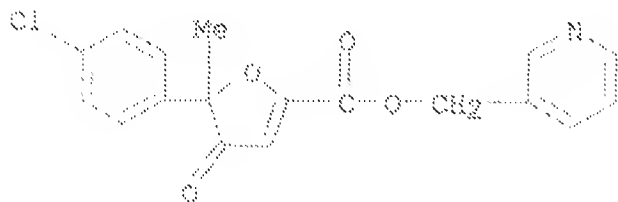
CMF C4 H4 O4

Double bond geometry as shown.



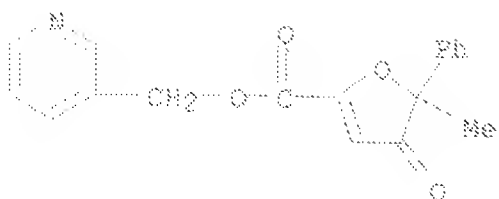
FN 72420-46-3 CAPLUS

CN 2-Furancarboxylic acid, 5-(4-chlorophenyl)-4,5-dihydro-5-methyl-4-oxo-,
3-pyridinylmethyl ester (CA INDEX NAME)



RN 72420-49-6 CAPLUS

CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl-,
3-pyridinylmethyl ester, hydrochloride (9CI) (CA INDEX NAME)

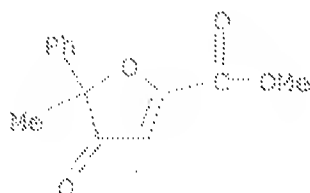


● HCl

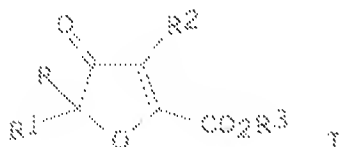
FN 72429-82-4 CAPLOS

CN 2-Furancarboxylic acid, 4,5-dihydro-5-methyl-4-oxo-5-phenyl-, methyl ester

(CA INDEX NAME)



GI



AB Furan derive, I (R, R1 = alkyl, cycloalkyl, alkoxy, Ph, etc.; R2 = H, alkyl; R3 = H, alkyl, etc.) and their salts, effective hypolipemics at

1.0

mmol/kg-day in rats, were prepared Thus, to a stirred suspension of

10.5 g

NaH in mineral oil was added 16 g di-Et oxalate and 16.4 g

3-hydroxy-3-phenyl-2-butanone in THF, the solution heated 18 h at 55-60°, cooled, and poured into H2O, NaOH added to pH 11, and the

mixture kept 24 h to give 20 g I (R = Me, R1 = Ph, R2 = R3 = H), which

10.4

g) was esterified with MeOH-H2SO4 to give 0.32 g Me ester (R = R3 =

Me, R1

= Ph, R2 = H). Similarly prepared were 9 addnl. I and salts.